

A Correlation Estimate for Quantum Many-Body Systems at Positive Temperature

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Abstract

We present an inequality that gives a lower bound on the expectation value of certain two-body interaction potentials in a general state on Fock space in terms of the corresponding expectation value for thermal equilibrium states of non-interacting systems and the difference in the free energy. This bound can be viewed as a rigorous version of first order perturbation theory for many-body systems at positive temperature. As an application, we give a proof of the first two terms in a high density (and high temperature) expansion of the free energy of jellium with Coulomb interactions, both in the fermionic and bosonic case. For bosons, our method works above the transition temperature (for the non-interacting gas) for Bose-Einstein condensation.

1 Introduction

Correlations play a crucial role in quantum-mechanical many-body systems. They result from interactions among the particles, and it is typically very difficult to obtain information about them in a mathematically rigorous fashion. Approximate theories are often arrived at by neglecting correlations,

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for instance in Hartree-Fock theory for fermions. For the problem of estimating the validity of such approximations, it is necessary to estimate the magnitude of correlations present in the state of the interacting system.

In [6], Graf and Solovej present a correlation estimate which is applicable for the study of this problem at zero temperature, i.e., for systems in their ground states. The inequality presented there is motivated by earlier correlation estimates by Bach [1] and Bach *et al.* [2]. Roughly speaking, it estimates the difference of the interaction energy in a general state and the ground state of a non-interacting system in terms of the difference of their one-particle density matrices. Moreover, at least in the case of fermions, the one-particle density matrix can be easily controlled in terms of the total kinetic energy. For bosonic systems, the situation is more complicated, and the correlation estimate in [6] is only applicable provided one can prove the existence of *Bose-Einstein condensation* — in general a very difficult task for interacting systems.

With the aid of the correlation estimate just mentioned, Graf and Solovej were able to derive the first two terms in a high density expansion of the ground state energy of fermionic jellium [6, Thm. 2] with Coulomb interactions. High density corresponds to small coupling, and hence the result can be viewed as rigorous estimate of the validity of first-order perturbation theory for this system.

In this paper, we present a method that is applicable to the aforementioned problem for systems at positive temperature. Unlike the situation for the ground state, the knowledge of the one-particle density matrix alone does not yield much information about correlations present in the state. As an additional input one needs to know that the *entropy* of the state is close to the maximal value possible for given one-particle density matrix; this maximum is attained by the corresponding *quasi-free state*. More precisely, we will estimate the difference of the interaction energy of a general state and the thermal equilibrium state of a non-interacting system in terms of the *relative entropy* of these two states. This relative entropy is related to the difference in free energy. Our result applies to fermions at any temperature, and to bosons above the critical temperature (for the non-interacting gas) for Bose-Einstein condensation.

Our main correlation estimate is stated in Theorem 3 in Section 3. Before describing it in detail, we present an application of the inequality to (fermionic or bosonic) jellium with Coulomb interactions at positive temperature. We will derive the first two terms in a high density (and high temperature) expansion of the free energy. In the fermionic case, this result can be viewed as the positive temperature analogue of Theorem 2 in [6].

Our estimate is general enough to be applicable to a wide range of possible interparticle interactions. The two-body potential is required to be positive definite and, in particular, to be decomposable into characteristic functions of balls. In the case of the Coulomb potential, such a decomposition was first used in [5]. The study in [7] provides a criterion for the possibility of such a decomposition for general radial functions, and thus provides many examples of interaction potentials which our method applies to.

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2 Jellium

Jellium is a model of a charged gas of either fermions or bosons, moving in a uniformly charged background. We assume that the whole system is neutral (in a sense to be made precise below) and contained in a (three-dimensional) cubic box of side length L , which we denote by Λ . We work in the grand-canonical ensemble, i.e., in the (anti-)symmetric Fock space over the one-particle space $\mathcal{H} = L^2(\Lambda; \mathbb{C}^n)$. Here, $n \geq 1$ denotes the number of internal degrees of freedom, corresponding to particles of spin $(n-1)/2$.

We denote by Δ the Laplacian on Λ with Dirichlet boundary conditions. We choose units such that $\hbar = 1$ and $2m = 1$, with m denoting the particle mass. For $\varrho > 0$ the background density and $\alpha > 0$ the square of the particle charge, the Hamiltonian on Fock space is

$$H = H_0 + \alpha W, \quad (2.1)$$

where, in each N -particle sector,

$$H_0 = - \sum_{i=1}^N \Delta_i \quad (2.2)$$

and

$$W = - \sum_{i=1}^N \varrho \int_{\Lambda} dy \frac{1}{|x_i - y|} + \sum_{i < j} \frac{1}{|x_i - x_j|} + \frac{1}{2} \varrho^2 \int_{\Lambda \times \Lambda} dy_1 dy_2 \frac{1}{|y_1 - y_2|}. \quad (2.3)$$

The last constant corresponds to the electrostatic energy of the background charge and is added to ensure the existence of a proper thermodynamic limit.

The quantity of interest is the free energy per unit volume at temperature $T = \beta^{-1}$, given by

$$f^{\text{F,B}}(\beta, \varrho, \alpha) = - \lim_{L \rightarrow \infty} \frac{1}{\beta|\Lambda|} \ln \text{Tr} \exp[-\beta H]. \quad (2.4)$$

Here, Tr denotes the trace either over the fermionic (F) or bosonic (B) Fock space. Existence of the thermodynamic limit in (2.4) was shown by Lieb and Narnhofer in [10]. There it was also shown that one would obtain the same result in the canonical ensemble with charge neutrality, i.e., fixing N to be $\varrho|\Lambda|$. In particular, in our grand-canonical setting it is not necessary to enforce the charge neutrality $N = \varrho|\Lambda|$ explicitly, it will be automatically satisfied (for the average particle number).

There are three length scales in this problem; the mean particle distance $\varrho^{-1/3}$, the thermal wavelength $\beta^{1/2}$, and the inverse coupling constant α^{-1} . Hence, by simple scaling,

$$f^{\text{F,B}}(\beta, \varrho, \alpha) = \varrho^{5/3} f^{\text{F,B}}(\beta \varrho^{2/3}, 1, \alpha \varrho^{-1/3}). \quad (2.5)$$

We are interested in the high density (and high temperature) asymptotics; more precisely, in large ϱ for fixed $\beta \varrho^{2/3}$ (and fixed α). By the scaling property (2.5), this corresponds to a limit of small coupling.

For the statement of our main results, we will distinguish between the fermionic and bosonic cases.

2.1 Fermions

Let $f_0^{\text{F}}(\beta, \varrho)$ denote the free energy (per unit volume) of a non-interacting gas of spin $(n-1)/2$ fermions, at inverse temperature β and average density ϱ . It is given by

$$f_0^{\text{F}}(\beta, \varrho) = \sup_{\mu \in \mathbb{R}} \left\{ \mu \varrho - \frac{n}{(2\pi)^3 \beta} \int_{\mathbb{R}^3} dp \ln \left(1 + e^{-\beta(p^2 - \mu)} \right) \right\}. \quad (2.6)$$

The supremum in (2.6) is attained uniquely at some $\mu = \mu_0^{\text{F}}(\beta, \varrho)$. We denote the fugacity by $z = e^{\beta\mu}$ for this value of μ . Note that z depends only on $\beta \varrho^{2/3}$. Let

$$\gamma_0^{\text{F}}(p) = \frac{1}{z^{-1} e^{\beta p^2} + 1}, \quad (2.7)$$

and let $\tilde{\gamma}_0^{\text{F}}(x) = (2\pi)^{-3} \int dp \gamma_0^{\text{F}}(p) e^{ipx}$ denote its inverse Fourier transform. Note that $n \tilde{\gamma}_0^{\text{F}}(0) = \varrho$.

THEOREM 1 (High Density Asymptotics for Fermions). *As $\varrho \rightarrow \infty$ and $\beta \rightarrow 0$,*

$$f^F(\beta, \varrho, \alpha) = f_0^F(\beta, \varrho) - \frac{\alpha n}{2} \int_{\mathbb{R}^3} dx \frac{|\tilde{\gamma}_0^F(x)|^2}{|x|} - o(\varrho^{4/3}), \quad (2.8)$$

with $0 \leq o(\varrho^{4/3}) \leq C(\beta \varrho^{2/3}) \alpha \varrho^{4/3} (\alpha \varrho^{-1/3})^{1/48}$. Moreover, the function $C(\beta \varrho^{2/3})$ is uniformly bounded on compact intervals in $(0, \infty)$.

Note that, for fixed $\beta \varrho^{2/3}$ (and fixed α), the first term on the right side of (2.8) is $O(\varrho^{5/3})$, whereas the second term is $O(\varrho^{4/3})$. Theorem 1 is the positive temperature analogue of Theorem 2 in [6].

We remark that (2.8) actually holds uniformly in $\beta \varrho^{2/3}$ for bounded $1/(\beta \varrho^{2/3})$, with possibly a worse exponent in the error term than the one given in Theorem 1. I.e., it is uniform as the ground state is approached. This can be proved by supplementing our lower bound with a bound obtained with the method in [6] at very low temperatures. We do not give the details here, but refer the reader to [15] where a similar argument was given in the case of a dilute Fermi gas with short-range interactions.

2.2 Bosons

For bosons we have to restrict our attention to temperatures bigger than the critical temperature (for the non-interacting gas) or, equivalently, to $\varrho < \varrho_c(\beta) \equiv n(4\pi\beta)^{-3/2} \sum_{\ell \geq 1} \ell^{-3/2}$. Let $f_0^B(\beta, \varrho)$ denote the free energy (per unit volume) of a non-interacting gas of spin $(n-1)/2$ bosons, given by

$$f_0^B(\beta, \varrho) = \sup_{\mu < 0} \left\{ \mu \varrho + \frac{n}{(2\pi)^3 \beta} \int_{\mathbb{R}^3} dp \ln \left(1 - e^{-\beta(p^2 - \mu)} \right) \right\}. \quad (2.9)$$

For $\varrho < \varrho_c(\beta)$, the supremum in (2.9) is attained at $\mu = \mu_0^B(\beta, \varrho) < 0$. Denote the fugacity by $z = e^{\beta\mu} < 1$ for this value of μ . Again, z depends only on the dimensionless quantity $\beta \varrho^{2/3}$. Analogously to (2.7), let

$$\gamma_0^B(p) = \frac{1}{z^{-1} e^{\beta p^2} - 1}, \quad (2.10)$$

and let $\tilde{\gamma}_0^B(x) = (2\pi)^{-3} \int dp \gamma_0^B(p) e^{ipx}$ denote its inverse Fourier transform.

THEOREM 2 (High Density Asymptotics for Bosons). *As $\varrho \rightarrow \infty$ and $\beta \rightarrow 0$ (with $\beta \varrho^{2/3} < \beta \varrho_c(\beta)^{2/3}$),*

$$f^B(\beta, \varrho, \alpha) = f_0^B(\beta, \varrho) + \frac{\alpha n}{2} \int_{\mathbb{R}^3} dx \frac{|\tilde{\gamma}_0^B(x)|^2}{|x|} - o(\varrho^{4/3}), \quad (2.11)$$

with $0 \leq o(\varrho^{4/3}) \leq C(\beta\varrho^{2/3})\alpha\varrho^{4/3}(\alpha\varrho^{-1/3})^{1/48}$. Moreover, the function $C(\beta\varrho^{2/3})$ is uniformly bounded on compact intervals in $(0, \beta\varrho_c(\beta)^{2/3})$.

As in the fermionic case, the first term on the right side of (2.11) is $O(\varrho^{5/3})$, whereas the second term is $O(\varrho^{4/3})$. Note that the second term diverges as $\varrho \rightarrow \varrho_c(\beta)$. This shows that (2.11) can not hold uniformly as ϱ approaches the critical density, since $f^B(\beta, \varrho, \alpha) \leq f^B(\infty, \varrho, \alpha) \leq 0$ for any β and ϱ . At zero temperature, the leading term in the energy density as $\varrho \rightarrow \infty$ is actually $O(\varrho^{5/4})$ [4, 12]. In particular, first order perturbation theory (in the grand canonical ensemble) is not applicable below the critical temperature, due to the large fluctuations in particle number. These large fluctuations cannot be present in the interacting system, for any non-zero value of the coupling parameter α .

The key ingredient in the proof of Theorems 1 and 2 is a new correlation estimate, which we present next.

3 Correlation Estimate

In this section, we will describe our main correlation estimate, which will then be used in the proof of Theorems 1 and 2. For $\xi \in \mathbb{R}^3$ and $r > 0$, let $\chi_{r,\xi}$ denote the characteristic function of a ball of radius r centered at ξ . The function $\chi_{r,\xi}$ defines a projection operator on $L^2(\mathbb{R}^3; \mathbb{C}^n)$ and also, in a natural way, on the subspace $L^2(\Lambda; \mathbb{C}^n)$. Let $n_{r,\xi}$ denote the operator on Fock space that counts the number of particles in this ball, i.e., the second quantization of the projection $\chi_{r,\xi}$ on $\mathcal{H} = L^2(\Lambda; \mathbb{C}^n)$. Our correlation estimate concerns a lower bound on the expectation value of the number of pairs of particles inside a ball of radius r or, more precisely, on

$$\int_{\mathbb{R}^3} d\xi \operatorname{Tr} [n_{r,\xi} (n_{r,\xi} - 1) \Gamma] . \quad (3.1)$$

Here, Γ is a density matrix, i.e., a positive operator on Fock space with trace equal to one, defining the state of the system.

Let γ_0 denote the one-particle density matrix of a (grand-canonical) non-interacting (Fermi or Bose) gas at temperature $T = \beta^{-1}$, with chemical potential $\mu = \mu_0^{\text{F,B}}(\beta, \varrho)$, as defined after Eqs. (2.6) and (2.9), respectively. We choose *periodic* boundary conditions for γ_0 , which has the advantage of γ_0 having a constant density. Note that the choice of μ implies that $|\Lambda|\bar{\varrho} \equiv \operatorname{tr} \gamma_0 = |\Lambda|\varrho + o(|\Lambda|)$ in the thermodynamic limit. Here and in the following, we denote the trace over the one-particle space $\mathcal{H} = L^2(\Lambda; \mathbb{C}^n)$ by

tr, whereas the trace over Fock space is denoted by Tr. The kernel of γ_0 is given by

$$\gamma_0(x, \sigma; y, \tau) = \frac{1}{|\Lambda|} \sum_{p \in \frac{2\pi}{L}\mathbb{Z}^3} \gamma_0^{\text{F,B}}(p) e^{ip(x-y)} \delta_{\sigma, \tau}, \quad (3.2)$$

where $\gamma_0^{\text{F,B}}(p)$ is given in (2.7) and (2.10), respectively, and σ and τ label the spin states.

Let Γ_0 denote the quasi-free state on Fock space with one-particle density matrix γ_0 . It is the Gibbs state (at inverse temperature 1 and chemical potential 0) for a non-interacting system with one-particle Hamiltonian $\ln[(1 \mp \gamma_0)/\gamma_0]$. Here and in the following, \mp means $-$ for fermions and $+$ for bosons (and vice versa for \pm). We note that for $\Gamma = \Gamma_0$, the expression in (3.1) can be easily calculated. Namely, for any r and ξ ,

$$\text{Tr} [n_{r,\xi}(n_{r,\xi} - 1)\Gamma_0] = (\text{tr} [\chi_{r,\xi}\gamma_0])^2 \mp \text{tr} (\chi_{r,\xi}\gamma_0)^2. \quad (3.3)$$

Hence, after integration over ξ ,

$$\begin{aligned} & \int_{\mathbb{R}^3} d\xi \text{Tr} [n_{r,\xi}(n_{r,\xi} - 1)\Gamma_0] \\ &= \int_{\Lambda \times \Lambda} dx dy J_r(x - y) [\bar{\varrho}^2 \mp \sum_{\sigma} |\gamma_0(x, \sigma; y, \sigma)|^2], \end{aligned} \quad (3.4)$$

where we denoted $J_r(x) = \int dy \chi_{r,\xi}(y) \chi_{r,\xi}(x - y)$. (Note that J_r is independent of ξ .) Here, we have also used that γ_0 has a constant density $\bar{\varrho} = \sum_{\sigma} \gamma_0(x, \sigma; x, \sigma)$ for $x \in \Lambda$.

We want to show that for states Γ that are in some sense close to the state Γ_0 , the expectation value (3.1) is close to (3.4). A convenient way to characterize this “proximity” is the *relative entropy*: For two general states Γ and Υ on Fock space, the relative entropy is given by

$$S(\Gamma, \Upsilon) = \text{Tr} \Gamma (\ln \Gamma - \ln \Upsilon). \quad (3.5)$$

Note that $0 \leq S(\Gamma, \Upsilon) \leq \infty$. Although S does not define a metric, it measures the difference between two states in a certain sense. In particular, S dominates the trace norm. More precisely, $S(\Gamma, \Upsilon) \geq 2\|\Gamma - \Upsilon\|_1^2$ [14, Thm. 1.15].

Note that the relative entropy can also be interpreted as a difference in free energies. More precisely, if $\Upsilon = \exp(-\beta(H - F))$ for some $\beta > 0$, with $F = -\beta^{-1} \ln \text{Tr} \exp(-\beta H)$ the corresponding “free energy”, then

$$\beta^{-1} S(\Gamma, \Upsilon) = \text{Tr} [H\Gamma] + \beta^{-1} \text{Tr} \Gamma \ln \Gamma - F. \quad (3.6)$$

Note that $-\text{Tr} \Gamma \ln \Gamma$ is just the von-Neumann entropy of Γ . Hence the first two terms on the right side of (3.6) correspond to the free energy of Γ (with Hamiltonian and temperature determined by Υ), whereas F is the free energy of Υ .

Our main result estimates the difference of the expectation value (3.1) for Γ_0 and a general state Γ in terms of the relative entropy $S(\Gamma, \Gamma_0)$. More precisely, the following Theorem, which is the main new result of this work, holds.

THEOREM 3 (Main Correlation Estimate). *Let Γ_0 be given as above, with one-particle density matrix γ_0 and density $\bar{\varrho}$, and with $\mu \in \mathbb{R}$ for fermions and $\mu < 0$ for bosons. Let Γ be any other state on (fermionic or bosonic) Fock space. For any $2r \leq d \leq L/2$, we have that*

$$\begin{aligned} & \int_{\mathbb{R}^3} d\xi \text{Tr} [n_{r,\xi} (n_{r,\xi} - 1) \Gamma] \\ & \geq \int_{\Lambda \times \Lambda} dx dy J_r(x - y) [\bar{\varrho}^2 \mp \sum_{\sigma} |\gamma_0(x, \sigma; y, \sigma)|^2] \\ & \quad - C_z^{\text{F,B}} r^3 \bar{\varrho} (1 + r^3 \bar{\varrho}) |\Lambda|^{3/4} \left[d^3 (1 + \beta d^{-2}) S(\Gamma, \Gamma_0) + \beta^{1/2} d^{-1} |\Lambda| \right]^{1/4}. \end{aligned} \quad (3.7)$$

Here, $C_z^{\text{F,B}}$ are constants depending only on $z = e^{\beta\mu}$, which are uniformly bounded on compact intervals in $(0, \infty)$ and $(0, 1)$, respectively.

We emphasize again that, according to (3.4), the second line in (3.7) equals the first in the case $\Gamma = \Gamma_0$. Although the inequality (3.7) is not sharp in this case, the parameter d can be made very large to obtain an error with is, in the thermodynamic limit, of lower order than the volume. (The restriction $d \leq L/2$ in Theorem 3 is purely technical and could in principle be avoided by a slight modification of the proof. Since we are mainly concerned here with the application of (3.7) in the thermodynamic limit $L \rightarrow \infty$, we have refrained from doing so.)

Note that Theorem 3 gives an estimate on a “local” quantity, like the expectation value of the number of pairs of particles inside a small ball, in terms of a “global” quantity as the relative entropy. The *strong subadditivity* of entropy plays a crucial role in this estimate. Before we give the proof of Theorem 3, we show how it can be used to prove the applications to Coulomb systems stated in Theorems 1 and 2.

4 Proof of Theorems 1 and 2

We are going to treat the fermionic and bosonic case simultaneously, merely pointing out the differences if necessary. We start by deriving a lower bound on the free energy. Note that if Γ denotes the Gibbs state of H at temperature β^{-1} (and zero chemical potential), then charge neutrality (as proved in [10]) implies that

$$\lim_{L \rightarrow \infty} \frac{1}{|\Lambda|} \text{Tr } N \Gamma = \varrho \quad (4.1)$$

for any fixed β and $\alpha > 0$. Here, N denotes the number operator on Fock space. Application of the Peierls-Bogoliubov inequality then leads to the lower bound

$$f^{\text{F,B}}(\beta, \varrho, \alpha) \geq f_0^{\text{F,B}}(\beta, \varrho) + \alpha \limsup_{L \rightarrow \infty} \frac{1}{|\Lambda|} \text{Tr } W \Gamma. \quad (4.2)$$

To estimate the expectation value of W in the Gibbs state Γ , we will split the Coulomb potential into a long and short-range part.

4.1 Long-Range Part

We write the Coulomb potential as [5]

$$\frac{1}{|x - y|} = \frac{1}{\pi} \int_0^\infty dr \frac{1}{r^5} \int_{\mathbb{R}^3} d\xi \chi_{r,\xi}(x) \chi_{r,\xi}(y). \quad (4.3)$$

As in Section 3, $\chi_{r,\xi}$ denotes the characteristic function of a ball of radius r centered at $\xi \in \mathbb{R}^3$. We split the r -integration into a part $r \leq R$ and a part $r \geq R$ and, correspondingly, write

$$\frac{1}{|x - y|} = V_{<R}(x - y) + V_{>R}(x - y). \quad (4.4)$$

Note that $V_{<R}(x) = 0$ for $|x| \geq 2R$. For the long-range part $V_{>R}$, we note that it has a positive Fourier transform, as follows immediately from the decomposition (4.3). Hence we obtain the lower bound [17, 4.5.20]

$$\begin{aligned} \sum_{1 \leq i < j \leq N} V_{>R}(x_i - x_j) &\geq \sum_{i=1}^N \varrho \int_{\Lambda} dy V_{>R}(x_i - y) \\ &\quad - \frac{1}{2} \varrho^2 \int_{\Lambda \times \Lambda} dy_1 dy_2 V_{>R}(y_1 - y_2) - \frac{N}{2} V_{>R}(0). \end{aligned} \quad (4.5)$$

This estimate actually holds for any $\varrho > 0$. The last term equals $V_{>R}(0) = 4/(3R)$, and hence will be negligible if we choose $R \gg \varrho^{-1/3}$.

4.2 Short-Range Part

As in Section 3, let $n_{r,\xi}$ denote the operator that counts the number of particles in a ball of radius r centered at ξ , i.e., the second quantization of the projection $\chi_{r,\xi}$ on $\mathcal{H} = L^2(\mathbb{R}^3; \mathbb{C}^n)$. The expectation value of the short-range part $V_{<R}$ of the interparticle interaction in a state Γ on Fock space can be written as

$$\frac{1}{2\pi} \int_0^R dr \frac{1}{r^5} \int_{\mathbb{R}^3} d\xi \operatorname{Tr} [n_{r,\xi} (n_{r,\xi} - 1) \Gamma] . \quad (4.6)$$

For a lower bound, we can now apply our main correlation estimate, Theorem 3, to the expression (4.6) for any fixed r .

Recall that γ_0 denotes the one-particle density matrix of a non-interacting (Fermi or Bose) gas at inverse temperature β , with chemical potential $\mu = \mu_0^{\text{F,B}}(\beta, \varrho)$, and with periodic boundary conditions; Γ_0 denotes the corresponding quasi-free state on Fock space. Theorem 3 states that for any $2r \leq d \leq L/2$,

$$\begin{aligned} & \int_{\mathbb{R}^3} d\xi \operatorname{Tr} [n_{r,\xi} (n_{r,\xi} - 1) \Gamma] \\ & \geq \int_{\Lambda \times \Lambda} dx dy J_r(x - y) [\bar{\varrho}^2 \mp \sum_{\sigma} |\gamma_0(x, \sigma; y, \sigma)|^2] \\ & \quad - C_z^{\text{F,B}} r^3 \bar{\varrho} (1 + r^3 \bar{\varrho}) |\Lambda|^{3/4} \left[d^3 (1 + \beta d^{-2}) S(\Gamma, \Gamma_0) + \beta^{1/2} d^{-1} |\Lambda| \right]^{1/4} . \end{aligned} \quad (4.7)$$

For Γ the Gibbs state of H , an upper bound on $S(\Gamma, \Gamma_0)$ is, in fact, easy to obtain. Using the fact that the quadratic form domain of the Dirichlet Laplacian is contained in the quadratic form domain of the Laplacian on Λ with periodic boundary conditions, we can write

$$\begin{aligned} S(\Gamma, \Gamma_0) &= \beta \operatorname{Tr} (H_0 - \mu N) \Gamma + \operatorname{Tr} \Gamma \ln \Gamma \mp \operatorname{tr} \ln(1 \mp \gamma_0) \\ &= -\ln \operatorname{Tr} \exp[-\beta H] - \beta \mu \operatorname{Tr} N \Gamma - \beta \alpha \operatorname{Tr} W \Gamma \mp \operatorname{tr} \ln(1 \mp \gamma_0) . \end{aligned} \quad (4.8)$$

We now use the lower bound $W \geq -\text{const. } N |\Lambda| \varrho^{1/3}$ [10], as well as the fact that $|\Lambda|^{-1} \operatorname{Tr} N \Gamma \rightarrow \varrho$ in the thermodynamic limit, as explained in the beginning of this section. This leads to the estimate

$$S(\Gamma, \Gamma_0) \leq |\Lambda| \beta \left(f^{\text{F,B}}(\beta, \varrho, \alpha) - f_0^{\text{F,B}}(\beta, \varrho) \right) + \text{const. } \beta |\Lambda| \alpha \varrho^{4/3} + o(|\Lambda|) . \quad (4.9)$$

As the upper bound to the free energy in Section 4.4 shows, the first term is negative in the fermionic case and can thus be neglected for an upper bound. In the bosonic case, it is bounded above by $C_z \beta |\Lambda| \alpha \varrho^{4/3}$ for some constant depending only on z . This follows immediately from the upper bound leading to (2.11), together with simple scaling. (Note that C_z diverges as $z \rightarrow 1$). Hence, in general,

$$S(\Gamma, \Gamma_0) \leq C_z \beta |\Lambda| \alpha \varrho^{4/3} + o(|\Lambda|). \quad (4.10)$$

Here and in the following, we abuse the notation slightly and denote by C_z any expression that depends only on z (and is uniformly bounded on compact intervals in $(0, \infty)$ in the fermionic case and $(0, 1)$ in the bosonic case).

We insert the bound (4.10) into (4.7). Choosing $d = \beta^{-1/8} \alpha^{-1/4} \varrho^{-1/3}$ we thus obtain that, as long as $d \geq 2r$ (and $\alpha \varrho^{-1/3} \leq \text{const.}$),

$$\begin{aligned} & \int_{\mathbb{R}^3} d\xi \operatorname{Tr} [n_{r,\xi} (n_{r,\xi} - 1) \Gamma] \\ & \geq \int_{\Lambda \times \Lambda} dx dy J_r(x - y) [\varrho^2 \mp \sum_{\sigma} |\gamma_0(x, \sigma; y, \sigma)|^2] \\ & \quad - C_z r^3 \varrho (1 + r^3 \varrho) |\Lambda| \left(\beta^{5/2} \alpha \varrho^{4/3} \right)^{1/16} + o(|\Lambda|). \end{aligned} \quad (4.11)$$

Here, we have also used that $\bar{\varrho} = \varrho + o(1)$ as $L \rightarrow \infty$. Note that we are going to use this estimate in (4.6) only for $r \leq R$. Below we will choose $R \ll \beta^{-1/8} \alpha^{-1/4} \varrho^{-1/3}$, hence (4.11) will be applicable.

For a lower bound, we can restrict the r -integration in (4.6) to $R_0 \leq r \leq R$ for some $0 < R_0 < R$, and simply neglect the contribution from the $r \leq R_0$ part. A simple estimate, using that $\sum_{\sigma} |\gamma_0(x, \sigma; y, \sigma)|^2 \leq \bar{\varrho}^2$, shows that in the state Γ_0 this $r \leq R_0$ contribution is bounded above by $(2\pi)^{-1} |\Lambda| (4\pi/3)^2 \bar{\varrho}^2 R_0^2$. We then have

$$\begin{aligned} & \frac{1}{2\pi} \int_0^R dr \frac{1}{r^5} \int_{\mathbb{R}^3} d\xi \operatorname{Tr} [n_{r,\xi} (n_{r,\xi} - 1) \Gamma] \\ & \geq \frac{1}{2} \int_{\Lambda \times \Lambda} dx dy V_{<R}(x - y) [\varrho^2 \mp \sum_{\sigma} |\gamma_0(x, \sigma; y, \sigma)|^2] - |\Lambda| \frac{8\pi}{9} \varrho^2 R_0^2 \\ & \quad - C_z \varrho |\Lambda| \left(\frac{1}{R_0} + R^2 \varrho \right) (\alpha \varrho^{-1/3})^{1/16} + o(|\Lambda|). \end{aligned} \quad (4.12)$$

Here, we have used again that z is a function of $\beta \varrho^{2/3}$.

4.3 Final Lower Bound

For the one-body part containing $V_{<R}$ (i.e., the interaction with the background), we can use the simple lower bound

$$-\sum_{i=1}^N \varrho \int_{\Lambda} dx V_{<R}(x - x_i) \geq -N\varrho \int_{\mathbb{R}^3} dx V_{<R}(x). \quad (4.13)$$

In combination, (4.5), (4.12) and (4.13) yield, in the thermodynamic limit,

$$\begin{aligned} \liminf_{L \rightarrow \infty} \frac{1}{|\Lambda|} \text{Tr } W\Gamma \geq \mp \frac{n}{2} \int_{\mathbb{R}^3} dx V_{<R}(x) |\tilde{\gamma}_0^{\text{F,B}}(x)|^2 - \frac{2\varrho}{3R} - \frac{8\pi}{9} \varrho^2 R_0^2 \\ - C_z \varrho \left(\frac{1}{R_0} + R^2 \varrho \right) (\alpha \varrho^{-1/3})^{1/16}. \end{aligned} \quad (4.14)$$

In the fermionic case, we can simply use $V_{<R}(x) \leq |x|^{-1}$ for a lower bound. In the bosonic case, we write $V_{<R}(x) = |x|^{-1} - V_{>R}(x)$ and estimate (using $V_{>R}(x) \leq V_{>R}(0) = 4/(3R)$)

$$\frac{n}{2} \int_{\mathbb{R}^3} dx V_{>R}(x) |\tilde{\gamma}_0^{\text{B}}(x)|^2 \leq \frac{2n}{3R} (2\pi)^{-3} \int_{\mathbb{R}^3} dp |\gamma_0^{\text{B}}(p)|^2 \leq \frac{2\varrho}{3R} \frac{z}{1-z}. \quad (4.15)$$

With the choice $R = \varrho^{-1/3} (\alpha \varrho^{-1/3})^{-1/48}$ and $R_0 = 1/(R^2 \varrho)$ this yields

$$\liminf_{L \rightarrow \infty} \frac{1}{|\Lambda|} \text{Tr } W\Gamma \geq \mp \frac{n}{2} \int_{\mathbb{R}^3} \frac{|\tilde{\gamma}_0^{\text{F,B}}(x)|^2}{|x|} - C_z \varrho^{4/3} (\alpha \varrho^{-1/3})^{1/48} \quad (4.16)$$

for some constant C_z depending only on z . Inserting this bound into (4.2) finishes the proof of the lower bound.

4.4 Upper Bound

For the upper bound to the free energy, we use the variational principle, which states that

$$-\frac{1}{\beta} \ln \text{Tr } \exp[-\beta H] \leq \text{Tr } H\Gamma - \frac{1}{\beta} S(\Gamma) \quad (4.17)$$

for any state Γ on Fock space. Here, $S(\Gamma) = -\text{Tr } \Gamma \ln \Gamma$ denotes the von-Neumann entropy. We choose as a trial state Γ a quasi-free state with one-particle density matrix γ given by the kernel

$$\gamma(x, \sigma; y, \tau) = g(x)g(y)\tilde{\gamma}_0^{\text{F,B}}(x - y)\delta_{\sigma,\tau}. \quad (4.18)$$

Here, $0 \leq g(x) \leq 1$ is a continuously differentiable function with the property that $g(x) = 0$ for $x \notin \Lambda$, $g(x) = 1$ if $x \in \Lambda$ and $\text{dist}(x, \partial\Lambda) \geq R$, and $|\nabla g| \leq \text{const.} R^{-1}$. We shall choose the variational parameter R to satisfy $1/(L\varrho^{2/3}) \ll R \ll (L\varrho^2)^{-1/5}$ for large L .

The calculation of the energy of the state Γ is similar to the corresponding calculation in [6]. It is in fact simpler since the particle number does not have to be fixed.

Let $\varphi(x) = \sum_{\sigma} \gamma(x, \sigma; x, \sigma)$ denote the density of γ . A simple computation (compare with (3.3)–(3.4)), using the fact that Γ is a quasi-free state, yields

$$\text{Tr } W\Gamma = \frac{1}{2} \int_{\Lambda \times \Lambda} dx dy \frac{1}{|x - y|} [(\varphi(x) - \varrho)(\varphi(y) - \varrho) \mp \sum_{\sigma} |\gamma(x, \sigma; y, \sigma)|^2] . \quad (4.19)$$

Note that $\varphi(x) = \varrho(1 - g(x)^2)$ and hence, by definition, $\varphi(x) = \varrho$ if $x \in \Lambda$ and x is at least a distance R away from the boundary of Λ . Using the Hardy-Littlewood-Sobolev inequality [9, Thm. 4.3], it is easy to see that the first term on the right side of (4.19) is bounded from above by $\text{const.} \varrho^2 (L^2 R)^{5/3}$ and is thus negligible in the thermodynamic limit, if $R \ll (L\varrho^2)^{-1/5}$. In the fermionic case, the second term is bounded from above by

$$-\frac{n}{2} \int_{\Lambda \times \Lambda} dx dy \frac{1}{|x - y|} |\tilde{\gamma}_0^{\text{F}}(x - y)|^2 (1 - 2(1 - g(x)^2)) , \quad (4.20)$$

which yields the desired expression in the thermodynamic limit, provided $R \ll L$, which is amply satisfied for our choice of R . In the bosonic case, we can simply use $g \leq 1$ to obtain the desired bound.

The kinetic energy of Γ is given by

$$\begin{aligned} \text{Tr } H_0\Gamma &= -n\Delta\tilde{\gamma}_0^{\text{F,B}}(0) \int_{\mathbb{R}^3} dx g(x)^2 + \varrho \int_{\mathbb{R}^3} dx |\nabla g(x)|^2 \\ &\leq -n|\Lambda|\Delta\tilde{\gamma}_0^{\text{F,B}}(0) + \text{const.} \frac{\varrho L^2}{R} . \end{aligned} \quad (4.21)$$

Again, the first term is the desired expression, and the last term is negligible if $R \gg 1/(L\varrho^{2/3})$.

It remains to derive a lower bound on the entropy $S(\Gamma)$. We claim that

$$\begin{aligned} S(\Gamma) &\geq -\frac{n}{(2\pi)^3} \int_{\Lambda} dx g(x)^2 \\ &\quad \times \int_{\mathbb{R}^3} dp \left[\gamma_0^{\text{F,B}}(p) \ln \gamma_0^{\text{F,B}}(p) \pm \left(1 \mp \gamma_0^{\text{F,B}}(p) \right) \ln \left(1 \mp \gamma_0^{\text{F,B}}(p) \right) \right] , \end{aligned} \quad (4.22)$$

which gives the desired quantity as long as $R \ll L$. Inequality (4.22) follows from a variant of the Berezin-Lieb inequality [3, 8]. The one-particle density matrix (4.18) can be written as

$$\gamma = \sum_{\sigma} \int_{\mathbb{R}^3} dp \gamma_0^{\text{F,B}}(p) g|p, \sigma\rangle \langle p, \sigma|g, \quad (4.23)$$

where g denotes multiplication by $g(x)$, and $|p, \sigma\rangle$ denotes a plane wave with wave function $(2\pi)^{-3/2} \exp(ipx)$ and spin σ . Moreover, since Γ is a quasi-free state,

$$S(\Gamma) = \text{tr } s(\gamma), \quad (4.24)$$

where we denoted $s(t) = -t \ln t \mp (1 \mp t) \ln(1 \mp t)$ for $t \geq 0$. Note that s is a concave function, with $s(0) = 0$. Hence we can apply the Berezin-Lieb inequality, in the form proved in Thm. A1 in [16]. Noting that

$$\sum_{\sigma} \int_{\mathbb{R}^3} dp g|p, \sigma\rangle \langle p, \sigma|g = g^2 \leq 1, \quad (4.25)$$

as well as $\langle p, \sigma|g^2|p, \sigma\rangle = (2\pi)^{-3} \int dx g(x)^2$, this yields (4.22).

We conclude that

$$\begin{aligned} -\lim_{L \rightarrow \infty} \frac{1}{\beta|\Lambda|} \ln \text{Tr} \exp[-\beta H] &\leq \mp \frac{n\alpha}{2} \int_{\mathbb{R}^3} dx \frac{|\tilde{\gamma}_0^{\text{F,B}}(x)|^2}{|x|} - n\Delta \tilde{\gamma}_0^{\text{F,B}}(0) \\ &+ \frac{n}{(2\pi)^3 \beta} \int_{\mathbb{R}^3} dp \left[\gamma_0^{\text{F,B}}(p) \ln \gamma_0^{\text{F,B}}(p) \pm \left(1 \mp \gamma_0^{\text{F,B}}(p)\right) \ln \left(1 \mp \gamma_0^{\text{F,B}}(p)\right) \right]. \end{aligned} \quad (4.26)$$

The last two terms together are just $f_0^{\text{F,B}}(\beta, \varrho)$. We have thus established the desired upper bounds. This concludes the proof of Theorems 1 and 2.

5 Proof of Theorem 3

5.1 Localization of Relative Entropy

If X denotes a projection on the one-particle space \mathcal{H} , then states on the Fock space can be restricted to the Fock space over the subspace $X\mathcal{H}$ of \mathcal{H} . We denote such a restriction of a state Γ by Γ_X . Since $\chi_{r,\xi}$ defines a projection on $\mathcal{H} = L^2(\Lambda; \mathbb{C}^n)$, we can write

$$\text{Tr} [n_{r,\xi} (n_{r,\xi} - 1) \Gamma] = \text{Tr} [n_{r,\xi} (n_{r,\xi} - 1) \Gamma_{\chi_{r,\xi}}], \quad (5.1)$$

the latter trace being over the Fock space over $\chi_{r,\xi}\mathcal{H}$.

It is well known [14] that the relative entropy decreases under restriction. More precisely, for any two states Γ and Υ on Fock space,

$$S(\Gamma, \Upsilon) \geq S(\Gamma_X, \Upsilon_X). \quad (5.2)$$

This property is closely related to the strong subadditivity of the von-Neumann entropy [11, 13].

Let $\eta : \mathbb{R}^3 \mapsto \mathbb{R}$ be a function with the following properties:

- $\eta \in C^4(\mathbb{R}^3)$
- $\eta(0) = 1$, and $\eta(x) = 0$ for $|x| \geq 1$
- $\hat{\eta}(p) = \int dx \eta(x) e^{-ipx} \geq 0$ for all $p \in \mathbb{R}^3$.

We note that such a function (with any degree of regularity) can, for instance, be obtained by taking a smooth function of compact support, and convolving it with itself. The resulting function is then smooth, has compact support and positive Fourier transform. In our application, we need the existence of the fourth derivatives at the origin (see Eq. (5.30) below).

Given such a function η , we define $\eta_d(x) = \eta(x/d)$ and

$$\eta_d^{\text{per}}(x) = \sum_{j \in \mathbb{Z}^3} \eta_d(x + jL). \quad (5.3)$$

Note that η_d^{per} is a periodic function with period L and, since $L \geq 2d$ by assumption, we have that $\eta_d^{\text{per}} \leq 1$. Moreover, we define a one-particle density matrix γ_d on \mathcal{H} by the kernel

$$\gamma_d(x, \sigma; y, \tau) = \gamma_0(x, \sigma; y, \tau) \eta_d^{\text{per}}(x - y), \quad (5.4)$$

with γ_0 defined in (3.2). This defines a positive operator, with plane waves as eigenfunctions, and eigenvalues determined by the convolution of $\hat{\eta}_d$ and $\gamma_0^{\text{F,B}}(p)$.

If $[L/2d]$ denotes the largest integer $\leq L/2d$, define \bar{d} by $L/2\bar{d} = [L/2d]$. Then $d \leq \bar{d} \leq 2d$. For $0 \leq r \leq d/2$, let X_r denote the characteristic function of a collection of balls of radius r , separated by $2\bar{d}$:

$$X_r(x) = \sum_{\xi \in 2\bar{d}\mathbb{Z}^3} \chi_{r,\xi}(x) = \sum_{\xi \in 2\bar{d}\mathbb{Z}^3 \cap [0,L]^3} \chi_{r,\xi}^{\text{per}}(x), \quad (5.5)$$

where we denoted

$$\chi_{r,\xi}^{\text{per}}(x) = \sum_{j \in \mathbb{Z}^3} \chi_{r,\xi}(x + jL). \quad (5.6)$$

Note that the minimal distance between the balls is $2\bar{d} - 2r \geq d$. Hence

$$X_r \gamma_d X_r = \sum_{\xi \in 2\bar{d}\mathbb{Z}^3 \cap [0, L]^3} \chi_{r, \xi}^{\text{per}} \gamma_d \chi_{r, \xi}^{\text{per}}, \quad (5.7)$$

the off-diagonal terms vanish since $\eta_d(x) = 0$ for $|x| \geq d$. I.e., $X_r \gamma_d X_r$ is a direct sum of one-particle density matrices on $\chi_{r, \xi}^{\text{per}} \mathcal{H}$ for $\xi \in 2\bar{d}\mathbb{Z}^3 \cap [0, L]^3$.

Let Γ_d denote the quasi-free state on Fock space with one-particle density matrix γ_d , and let Γ denote any other state on Fock space. The characteristic function X_r defines a projection operator on the one-particle space $\mathcal{H} = L^2(\Lambda; \mathbb{C}^n)$. Hence the monotonicity of the relative entropy implies

$$S(\Gamma, \Gamma_d) \geq S(\Gamma_{X_r}, \Gamma_{d, X_r}), \quad (5.8)$$

where Γ_{X_r} and Γ_{d, X_r} denote the states restricted to the Fock space over $X_r \mathcal{H}$, respectively. Note that the one-particle density matrix of the quasi-free state Γ_{d, X_r} is given by $X_r \gamma_d X_r$. Hence (5.7) shows that Γ_{d, X_r} can be written as a product of states on the Fock spaces over the one-particle spaces $\chi_{r, \xi}^{\text{per}} \mathcal{H}$ for $\xi \in 2\bar{d}\mathbb{Z}^3 \cap [0, L]^3$. Under this condition S is superadditive, as follows easily from subadditivity of the von-Neumann entropy [14]. More precisely,

$$S(\Gamma, \Gamma_d) \geq S(\Gamma_{X_r}, \Gamma_{d, X_r}) \geq \sum_{\xi \in 2\bar{d}\mathbb{Z}^3 \cap [0, L]^3} S(\Gamma_{\chi_{r, \xi}^{\text{per}}}, \Gamma_{d, \chi_{r, \xi}^{\text{per}}}). \quad (5.9)$$

We can repeat the argument above with a projector defined by the multiplication operator $X_r(x + a)$ for some vector $a \in [0, 2\bar{d}]^3$. Averaging over a then yields

$$\begin{aligned} S(\Gamma, \Gamma_d) &\geq \frac{1}{(2\bar{d})^3} \int_{[0, 2\bar{d}]^3} da \sum_{\xi \in 2\bar{d}\mathbb{Z}^3 \cap [0, L]^3} S(\Gamma_{\chi_{r, \xi+a}^{\text{per}}}, \Gamma_{d, \chi_{r, \xi+a}^{\text{per}}}) \\ &= \frac{1}{(2\bar{d})^3} \int_{\Lambda} d\xi S(\Gamma_{\chi_{r, \xi}^{\text{per}}}, \Gamma_{d, \chi_{r, \xi}^{\text{per}}}). \end{aligned} \quad (5.10)$$

Remark. We emphasize that in order to obtain the superadditivity of the relative entropy leading to (5.9), we have used the fact that $\Gamma_{d, X_r} = \bigotimes_{\xi} \Gamma_{d, \chi_{r, \xi}^{\text{per}}}$. Our estimate applies to any density matrix having this property. For a general state, however, it will be difficult to check this property; in the case of a quasi-free state considered here, it simply translates to the vanishing of off-diagonal terms in the one-particle density matrix (more precisely, the validity of (5.7)).

5.2 Upper Bound on Relative Entropy with Cutoff

In the previous subsection, we have shown how to localize relative entropy in the case when the second argument is a state that has been cut off in such away as to avoid correlations between balls of a certain distance. In the following, we will quantify the effect of this cut-off on the relative entropy.

If Γ_γ denotes the quasi-free state with one-particle density matrix γ , and Υ is any other state on Fock space, then $S(\Upsilon, \Gamma_\gamma)$ is convex in γ . This follows from operator-concavity of the logarithm and $S(\Upsilon, \Gamma_\gamma) = \text{Tr } \Upsilon \ln \Upsilon - \text{tr } \omega \ln \gamma \mp \text{tr } (1 \mp \omega) \ln(1 \mp \gamma)$, where ω denotes the one-particle density matrix of Υ . Note that γ_d can be written as a convex combination of the form

$$\gamma_d = \frac{1}{|\Lambda|} \sum_{q \in \frac{2\pi}{L}\mathbb{Z}^3} \hat{\eta}_d(q) \gamma_{0,q} \quad (5.11)$$

where $\gamma_{0,q}$ is defined by the kernel

$$\gamma_{0,q}(x, \sigma; y, \tau) = \frac{1}{|\Lambda|} \sum_{p \in \frac{2\pi}{L}\mathbb{Z}^3} \frac{1}{2} \left[\gamma_0^{\text{F,B}}(p+q) + \gamma_0^{\text{F,B}}(p-q) \right] e^{ip(x-y)} \delta_{\sigma,\tau}. \quad (5.12)$$

Hence convexity implies that, for any state Γ ,

$$S(\Gamma, \Gamma_d) \leq \frac{1}{|\Lambda|} \sum_{q \in \frac{2\pi}{L}\mathbb{Z}^3} \hat{\eta}_d(q) S(\Gamma, \Gamma_{0,q}), \quad (5.13)$$

where $\Gamma_{0,q}$ denotes the quasi-free state corresponding to the one-particle density matrix $\gamma_{0,q}$.

Recall that Γ_0 denotes the quasi-free state on Fock space with one-particle density matrix γ_0 given in (3.2), i.e., $\Gamma_0 \equiv \Gamma_{0,0}$. We claim that, for any $t > 0$,

$$S(\Gamma, \Gamma_{0,q}) \leq (1+t^{-1}) S(\Gamma, \Gamma_0) + \text{tr } (h_q - h_0) \left(\frac{1}{e^{(1+t)h_0 - th_q} \pm 1} - \frac{1}{e^{h_q} \pm 1} \right), \quad (5.14)$$

where $h_q = \ln[(1 \mp \gamma_{0,q})/\gamma_{0,q}]$. In the Bose case, we have to assume that $(1+t)h_0 - th_q > 0$, which is satisfied for t small enough, as our estimates in Lemma 2 below will show. Inequality (5.14) follows from the two inequalities (where γ denotes the one-particle density matrix of Γ)

$$\begin{aligned} & \text{tr } \gamma((1+t)h_0 - th_q) + \text{Tr } \Gamma \ln \Gamma \\ & \geq \mp \text{tr } \ln \left(1 \pm e^{-(1+t)h_0 + th_q} \right) \\ & \geq \mp \text{tr } \ln \left(1 \pm e^{-h_0} \right) + t \text{tr } (h_0 - h_q) [e^{(1+t)h_0 - th_q} \pm 1]^{-1} \end{aligned} \quad (5.15)$$

and

$$\mp \text{tr} \ln \left(1 \pm e^{-h_q} \right) \geq \mp \text{tr} \ln \left(1 \pm e^{-h_0} \right) + \text{tr} (h_q - h_0) [e^{h_q} \pm 1]^{-1}. \quad (5.16)$$

Dividing (5.15) by t and adding (5.16) yields (5.14).

To estimate the last term in (5.14), we need the following simple lemmas, estimating the expression

$$h_q^{\text{F,B}}(p) = \ln \frac{2 \mp \gamma_0^{\text{F,B}}(p+q) \mp \gamma_0^{\text{F,B}}(p-q)}{\gamma_0^{\text{F,B}}(p+q) + \gamma_0^{\text{F,B}}(p-q)}. \quad (5.17)$$

Note that $h_0^{\text{F,B}}(p) = \beta(p^2 - \mu)$.

Lemma 1 (Fermions). *Let $D_z = \sup_{u>0} [zu/(e^u + z)]$. Then*

$$-2\beta q^2(3D_z + 2\beta p^2) \leq h_q^{\text{F}}(p) - h_0^{\text{F}}(p) \leq 2\beta q^2(1 + 2D_z). \quad (5.18)$$

Moreover,

$$\beta(q^2 - 2|pq|) \leq h_q^{\text{F}}(p) - h_0^{\text{F}}(p) \leq \beta(q^2 + 2|pq|) \quad (5.19)$$

independently of z .

Lemma 2 (Bosons). *Let $D_z = \sup_{u>0} [z^2 u e^u / (e^u - z)^2]$. Then*

$$-2\beta q^2(3D_z + 2\beta p^2) \leq h_q^{\text{B}}(p) - h_0^{\text{B}}(p) \leq \beta q^2. \quad (5.20)$$

Moreover,

$$h_q^{\text{B}}(p) - h_0^{\text{B}}(p) \geq \beta(q^2 - 2|pq|) \quad (5.21)$$

independently of z .

We defer the proof of Lemmas 1 and 2 to the appendix.

The last term in (5.14) is given by

$$n \sum_{p \in \frac{2\pi}{L} \mathbb{Z}^3} \left(h_q^{\text{F,B}}(p) - h_0^{\text{F,B}}(p) \right) \left(\frac{1}{e^{(1+t)h_0^{\text{F,B}}(p) - th_q^{\text{F,B}}(p)} \pm 1} - \frac{1}{e^{h_q^{\text{F,B}}(p)} \pm 1} \right). \quad (5.22)$$

A simple estimate on the derivative of the last term in brackets with respect to $h_0^{\text{F,B}}(p) - h_q^{\text{F,B}}(p)$ shows that (5.22) is bounded above by

$$n(1+t)C_z \sum_{p \in \frac{2\pi}{L} \mathbb{Z}^3} \left(h_q^{\text{F,B}}(p) - h_0^{\text{F,B}}(p) \right)^2 \sup_{-1 \leq s \leq t} \frac{1}{e^{(1+s)h_0^{\text{F,B}}(p) - sh_q^{\text{F,B}}(p)} \pm 1}, \quad (5.23)$$

where $C_z = 1$ for fermions and $C_z = (1 - z)^{-1}$ for bosons. (Here we have used that $1 + \gamma_0^B(p) \leq (1 - z)^{-1}$.) The upper bounds in (5.18) and (5.20) show that, for $0 \leq s \leq t$,

$$(1 + s)h_0^{F,B}(p) - sh_q^{F,B}(p) \geq \begin{cases} h_0^F(p) - 2t\beta q^2(1 + 2D_z) & \text{for fermions,} \\ h_0^B(p) - t\beta q^2 & \text{for bosons.} \end{cases} \quad (5.24)$$

We choose $t = \min\{1, (2\beta q^2(1 + 2D_z))^{-1}\}$ in the fermionic case, and $t = \min\{1, -\mu/(2q^2)\}$ in the bosonic case. With this choice, (5.24) becomes

$$(1 + s)h_0^{F,B}(p) - sh_q^{F,B}(p) \geq \begin{cases} \beta(p^2 - \mu) - 1 & \text{for fermions,} \\ \beta(p^2 - \mu/2) & \text{for bosons} \end{cases} \quad (5.25)$$

for $0 \leq s \leq t$. For $-1 \leq s \leq 0$ we use the lower bounds in (5.19) and (5.21), respectively. It is then easy to see that in this case

$$(1 + s)h_0^{F,B}(p) - sh_q^{F,B}(p) \geq \beta [\min\{p^2, (p - q)^2, (p + q)^2\} - \mu] . \quad (5.26)$$

Applying the bounds (5.26) and (5.25) to the denominator in (5.23) and using (5.18) and (5.20), respectively, to bound the expression $(h_0^{F,B}(p) - h_q^{F,B}(p))^2$ from above, we obtain that

$$(5.22) \leq C_z |\Lambda| \beta^{1/2} q^4 \quad (5.27)$$

as long as $\beta q^2 \leq \text{const}$. Here we have also used that $t \leq 1$ by definition. (Again, as in Section 4, we abuse the notation slightly and denote by C_z any expression that depends only on z .)

It remains to show that (5.27) holds also for large values of βq^2 . To do this, we can go back to (5.22) and apply the bounds above directly to this term. In case $h_q^{F,B}(p) \geq h_0^{F,B}(p)$, we use (5.25) (with $s = t$) as well as the upper bounds in (5.18) and (5.20). For the case $h_q^{F,B}(p) \leq h_0^{F,B}(p)$, we use (5.26) and the lower bounds in (5.19) and (5.21). We then split the sum into three regions according to where the minimum in (5.26) is attained, and change variables from p to $p - q$ or $p + q$, respectively. In this way we see that

$$(5.22) \leq C_z |\Lambda| \beta^{-1} |q| \left(1 + \beta^{1/2} |q|\right) \quad (5.28)$$

for any value of q . Hence, in particular, (5.27) holds for all q .

We have thus shown that

$$S(\Gamma, \Gamma_{0,q}) \leq 2(1 + C'_z \beta q^2) S(\Gamma, \Gamma_0) + C_z |\Lambda| \beta^{1/2} q^4, \quad (5.29)$$

with $C'_z = 1 + 2D_z$ for fermions and $C'_z = -1/\ln z$ for bosons. We insert this bound into (5.13) and sum over q . We can use

$$\frac{1}{|\Lambda|} \sum_{q \in \frac{2\pi}{L}\mathbb{Z}^3} \hat{\eta}_d(q) q^4 = \Delta^2 \eta(0) d^{-4} \quad (5.30)$$

and similarly for q^4 replaced by q^2 . This leads to the result that, irrespective of whether we consider Fermi or Bose symmetry,

$$S(\Gamma, \Gamma_d) \leq C_z \left[(1 + \beta d^{-2}) S(\Gamma, \Gamma_0) + |\Lambda| \frac{\beta^{1/2}}{d^4} \right], \quad (5.31)$$

with C_z a constant depending only on $z = e^{\beta\mu}$.

5.3 Final Steps in the Proof

If $n_{r,\xi}$ denotes the operator that counts the number of particles in a ball of radius r centered at ξ , we want a lower bound on the expression

$$\int_{\mathbb{R}^3} d\xi \operatorname{Tr} [n_{r,\xi} (n_{r,\xi} - 1) \Gamma_{\chi_{r,\xi}}]. \quad (5.32)$$

For a lower bound, we can replace the positive operator $n_{r,\xi}(n_{r,\xi} - 1)$ by $f_K(n_{r,\xi}(n_{r,\xi} - 1))$, where

$$f_K(t) = \begin{cases} t & \text{for } t \leq K \\ K & \text{for } t > K \end{cases} \quad (5.33)$$

for some $K > 0$ to be determined. Then

$$\begin{aligned} \operatorname{Tr} [n_{r,\xi} (n_{r,\xi} - 1) \Gamma_{\chi_{r,\xi}}] &\geq \operatorname{Tr} [f_K(n_{r,\xi}(n_{r,\xi} - 1)) \Gamma_{\chi_{r,\xi}}] \\ &\geq \operatorname{Tr} [f_K(n_{r,\xi}(n_{r,\xi} - 1)) \Gamma_{d,\chi_{r,\xi}}] \\ &\quad - K \|\Gamma_{\chi_{r,\xi}} - \Gamma_{d,\chi_{r,\xi}}\|_1. \end{aligned} \quad (5.34)$$

Next we note that $t - f_K(t) = [t - K]_+ \leq t^2/(4K)$, and hence

$$\begin{aligned} &\operatorname{Tr} [f_K(n_{r,\xi}(n_{r,\xi} - 1)) \Gamma_{d,\chi_{r,\xi}}] \\ &\geq \operatorname{Tr} [n_{r,\xi}(n_{r,\xi} - 1) \Gamma_{d,\chi_{r,\xi}}] - \frac{1}{4K} \operatorname{Tr} [n_{r,\xi}^2 (n_{r,\xi} - 1)^2 \Gamma_{d,\chi_{r,\xi}}]. \end{aligned} \quad (5.35)$$

Note that $\Gamma_{d,\chi_{r,\xi}}$ is a quasi-free state. Hence (compare with (3.3)–(3.4))

$$\begin{aligned} & \int_{\mathbb{R}^3} d\xi \operatorname{Tr} [n_{r,\xi}(n_{r,\xi} - 1)\Gamma_{d,\chi_{r,\xi}}] \\ &= \int_{\Lambda \times \Lambda} dx dy J_r(x - y) [\bar{\varrho}^2 \mp \sum_{\sigma} |\gamma_d(x, \sigma; y, \sigma)|^2] . \end{aligned} \quad (5.36)$$

Moreover, the last term in (5.35) is easy to estimate. Since $\Gamma_{d,\chi_{r,\xi}}$ is quasi-free, it can be explicitly expressed in terms of $\chi_{r,\xi}\gamma_d\chi_{r,\xi}$. A simple estimate then yields, in the fermionic case,

$$\operatorname{Tr} [n_{r,\xi}^2(n_{r,\xi} - 1)^2\Gamma_{d,\chi_{r,\xi}}] \leq (\operatorname{tr} [\chi_{r,\xi}\gamma_d])^2 (\operatorname{tr} [\chi_{r,\xi}\gamma_d] + 2)^2 . \quad (5.37)$$

In the bosonic case, we obtain

$$\operatorname{Tr} [n_{r,\xi}^2(n_{r,\xi} - 1)^2\Gamma_{d,\chi_{r,\xi}}] \leq 24 (\operatorname{tr} [\chi_{r,\xi}\gamma_d])^2 (\operatorname{tr} [\chi_{r,\xi}\gamma_d] + \frac{1}{2})^2 . \quad (5.38)$$

Note that $\operatorname{tr} [\chi_{r,\xi}\gamma_d] = 4\pi r^3 \bar{\varrho}/3$ as long as Λ contains the ball of radius r centered at ξ , since γ_d has a constant density $\bar{\varrho}$. For any ξ and r we have $\operatorname{tr} [\chi_{r,\xi}\gamma_d] \leq 4\pi r^3 \bar{\varrho}/3$. Integrating over ξ thus yields

$$\int_{\mathbb{R}^3} d\xi \operatorname{Tr} [n_{r,\xi}^2(n_{r,\xi} - 1)^2\Gamma_{d,\chi_{r,\xi}}] \leq \operatorname{const.} |\Lambda| (r^3 \bar{\varrho})^2 (1 + r^3 \bar{\varrho})^2 . \quad (5.39)$$

To estimate the last term in (5.34), we first note that $\|\Gamma_{\chi_{r,\xi}} - \Gamma_{d,\chi_{r,\xi}}\|_1^2 \leq 2S(\Gamma_{\chi_{r,\xi}}, \Gamma_{d,\chi_{r,\xi}})$ [14, Thm. 1.15]. Using Schwarz's inequality for the ξ -integration yields

$$\int_{\mathbb{R}^3} d\xi \|\Gamma_{\chi_{r,\xi}} - \Gamma_{d,\chi_{r,\xi}}\|_1 \leq \sqrt{2}(L + 2r)^{3/2} \left(\int_{\mathbb{R}^3} d\xi S(\Gamma_{\chi_{r,\xi}}, \Gamma_{d,\chi_{r,\xi}}) \right)^{1/2} . \quad (5.40)$$

Here we have also used the fact that the integrand is zero if the distance between ξ and Λ is bigger than r , since there are no particles outside Λ and hence both restricted states are the Fock space vacuum in this case. To estimate the last term in (5.40), we would like to use (5.10). We note that, again by monotonicity of the relative entropy, $S(\Gamma_{\chi_{r,\xi}}, \Gamma_{d,\chi_{r,\xi}}) \leq S(\Gamma_{\chi_{r,\xi}^{\text{per}}}, \Gamma_{d,\chi_{r,\xi}^{\text{per}}})$. The latter quantity is periodic in ξ , with period L . Moreover, since $r \leq L/2$ by assumption, the cube of side length $L + 2r$ is contained within 3^3 copies of Λ , and hence

$$\int_{\mathbb{R}^3} d\xi S(\Gamma_{\chi_{r,\xi}}, \Gamma_{d,\chi_{r,\xi}}) \leq 3^3 \int_{\Lambda} d\xi S(\Gamma_{\chi_{r,\xi}^{\text{per}}}, \Gamma_{d,\chi_{r,\xi}^{\text{per}}}) . \quad (5.41)$$

Using (5.10) this yields

$$\int_{\mathbb{R}^3} d\xi \|\Gamma_{\chi_{r,\xi}} - \Gamma_{d,\chi_{r,\xi}}\|_1 \leq 4(L+2r)^{3/2} (3\bar{d})^{3/2} S(\Gamma, \Gamma_d)^{1/2}. \quad (5.42)$$

Note that $(L+2r) \leq (3/2)|\Lambda|^{1/3}$ since $2r \leq L/2$ by assumption, as well as $\bar{d} \leq 2d$.

Collecting all the terms and optimizing over K , we obtain the lower bound

$$\begin{aligned} & \int_{\mathbb{R}^3} d\xi \operatorname{Tr} [n_{r,\xi} (n_{r,\xi} - 1) \Gamma] \\ & \geq \int_{\Lambda \times \Lambda} dx dy J_r(x-y) [\bar{\varrho}^2 \mp \sum_{\sigma} |\gamma_d(x, \sigma; y, \sigma)|^2] \\ & \quad - \operatorname{const.} r^3 \bar{\varrho} (1 + r^3 \bar{\varrho}) |\Lambda|^{3/4} d^{3/4} S(\Gamma, \Gamma_d)^{1/4}. \end{aligned} \quad (5.43)$$

Note that $|\gamma_d(x, \sigma; y, \sigma)| \leq |\gamma_0(x, \sigma; y, \sigma)|$ because of (5.4) and the fact that $|\eta_d^{\text{per}}| \leq 1$. Hence (5.43), together with (5.31), proves the Theorem in the fermionic case.

In the bosonic case, we have to estimate, in addition, the term

$$\sum_{\sigma} \int_{\Lambda \times \Lambda} dx dy J_r(x-y) |\gamma_0(x, \sigma; y, \sigma)|^2 (1 - \eta_d^{\text{per}}(x-y)^2). \quad (5.44)$$

We use that $J_r(x) \leq (4\pi/3)r^3$ and $|\gamma_0(x, \sigma; y, \sigma)| \leq \bar{\varrho}/n$. Moreover, we can estimate $\eta_d^{\text{per}}(x)^2 \geq 1 - \operatorname{const.} (x/d)^{\nu}$ for any $0 < \nu \leq 2$. Choosing $\nu = 1/4$ we obtain the bound

$$(5.44) \leq \operatorname{const.} r^3 \bar{\varrho} d^{-1/4} \int_{\Lambda \times \Lambda} dx dy |\gamma_0(x, \sigma; y, \sigma)| |x-y|^{1/4}. \quad (5.45)$$

By simple scaling, the integral is bounded above by $C_z |\Lambda| \beta^{1/8}$ for some z -dependent constant. Hence the error term (5.44) can be absorbed into the error terms already present in (5.43), merely adjusting the constant.

This finishes the proof of Theorem 3.

A Appendix

Proof of Lemmas 1 and 2. We first prove (5.19) and (5.21). Since both $x \mapsto \ln[(2-x)/x]$ and $x \mapsto \ln[(2+x)/x]$ are monotone decreasing (for $0 < x < 2$ and $x > 0$, respectively), we can obtain upper and lower bounds on $h_q^{\text{F,B}}(p)$

by replacing $\gamma_0^{\text{F,B}}(p+q)$ and $\gamma_0^{\text{F,B}}(p-q)$ by the minimal and maximal value of these two expressions, respectively. This yields (5.19) and (5.21).

The upper bound in (5.20) follows immediately from convexity of the map $x \mapsto \ln[(2+x)/x]$ for $x > 0$.

The proof of (5.18) and the lower bound in (5.20) is a bit more tedious, but elementary. For convenience we set $\beta = 1$, the correct β -dependence follows easily by scaling. For $0 \leq \lambda \leq 1$, we define $f(\lambda) = h_{\lambda q}^{\text{F,B}}(p)$. Note that $f'(0) = 0$ and hence

$$h_q^{\text{F,B}}(p) - h_0^{\text{F,B}}(p) = f(1) - f(0) = \int_0^1 d\lambda (1-\lambda) f''(\lambda). \quad (\text{A.1})$$

To calculate $f''(\lambda)$ it is useful to note that

$$q \nabla \gamma_0^{\text{F,B}}(p) = -2pq \gamma_0^{\text{F,B}}(p) (1 \mp \gamma_0^{\text{F,B}}(p)) \quad (\text{A.2})$$

and

$$\begin{aligned} (q \nabla)^2 \gamma_0^{\text{F,B}}(p) &= -2q^2 \gamma_0^{\text{F,B}}(p) (1 \mp \gamma_0^{\text{F,B}}(p)) \\ &\quad + 8(pq)^2 \gamma_0^{\text{F,B}}(p) (1 \mp \gamma_0^{\text{F,B}}(p)) \left(\frac{1}{2} \mp \gamma_0^{\text{F,B}}(p)\right). \end{aligned} \quad (\text{A.3})$$

Denoting $p_{\pm} = p \pm \lambda q$ and $\gamma_{\pm} = \gamma_0^{\text{F,B}}(p_{\pm})$, we therefore have

$$\begin{aligned} f''(\lambda) &= \left[-\frac{1}{(2 \mp \gamma_+ \mp \gamma_-)^2} + \frac{1}{(\gamma_+ + \gamma_-)^2} \right] \\ &\quad \times \left(2p_+ q \gamma_+ (1 \mp \gamma_+) - 2p_- q \gamma_- (1 \mp \gamma_-) \right)^2 \\ &\quad - \left[\pm \frac{1}{2 \mp \gamma_+ \mp \gamma_-} + \frac{1}{\gamma_+ + \gamma_-} \right] \left(-2q^2 \gamma_+ (1 \mp \gamma_+) - 2q^2 \gamma_- (1 \mp \gamma_-) \right. \\ &\quad \left. + 8(p_+ q)^2 \gamma_+ (1 \mp \gamma_+) \left(\frac{1}{2} \mp \gamma_+\right) + 8(p_- q)^2 \gamma_- (1 \mp \gamma_-) \left(\frac{1}{2} \mp \gamma_-\right) \right). \end{aligned} \quad (\text{A.4})$$

Rearranging the various terms we can write

$$\begin{aligned}
f''(\lambda) = & \frac{\pm 4}{\gamma_+ + \gamma_-} \left[(p_+q)^2 \gamma_+^2 (1 \mp \gamma_+) + (p_-q)^2 \gamma_-^2 (1 \mp \gamma_-) \right. \\
& \left. \mp \frac{\gamma_+ \gamma_-}{\gamma_+ + \gamma_-} \left(p_+q(1 \mp \gamma_+) + p_-q(1 \mp \gamma_-) \right)^2 \right] \\
& \mp \frac{4}{2 \mp \gamma_+ \mp \gamma_-} \left[(p_+q)^2 \gamma_+ (1 \mp \gamma_+)^2 + (p_-q)^2 \gamma_- (1 \mp \gamma_-)^2 \right. \\
& \left. \mp \frac{(1 \mp \gamma_+)(1 \mp \gamma_-)}{2 \mp \gamma_+ \mp \gamma_-} \left(p_+q \gamma_+ + p_-q \gamma_- \right)^2 \right] \\
& + \left[\pm \frac{1}{2 \mp \gamma_+ \mp \gamma_-} + \frac{1}{\gamma_+ + \gamma_-} \right] \left(2q^2 \gamma_+ (1 \mp \gamma_+) + 2q^2 \gamma_- (1 \mp \gamma_-) \right).
\end{aligned} \tag{A.5}$$

The term in the last line is positive and bounded above by $4q^2$, both in the fermionic and bosonic case. For an upper bound in the fermionic case, we use that $p_\pm^2 \gamma_\pm \leq D_z$, $|p_\pm| \gamma_\pm \leq \sqrt{D_z}$ as well as $0 \leq \gamma_\pm \leq 1$ to get $f''(\lambda) \leq 4q^2(1 + 2D_z)$. Similarly we can obtain a lower bound. Using that $p_+q + p_-q = 2pq$ in the second line in (A.5), a simple estimate yields $f''(\lambda) \geq -12q^2 D_z - 8p^2 q^2$ in the fermionic case. Using these bounds in (A.1) proves (5.18).

In the bosonic case, we only need to prove a lower bound on (A.5). Proceeding as above, this time using $p_\pm^2 \gamma_\pm (1 + \gamma_\pm) \leq D_z$ and $|p_\pm| \gamma_\pm \leq \sqrt{D_z}$ we obtain again $f''(\lambda) \geq -12q^2 D_z - 8p^2 q^2$. This finishes the proof of the lemmas. \blacksquare

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